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Publications: 313 peer reviewed, 53 reviews, books and non-peer reviewed  
H-index: Publons - 79 (85,000+ citations), Google Scholar - 98 (117,000+ citations)  
Outreach: 200+ invited lectures and workshops

### **Professional Experience**

2021-Now Associate Laboratory Director for Biosciences, Lawrence Berkeley Laboratory  
2015-2021 Division Director, Molecular Biophysics & Integrated Bioimaging, Lawrence Berkeley Laboratory  
2011-2021 Division Deputy for Biosciences, Advanced Light Source, Lawrence Berkeley Laboratory  
2009-Now Laboratory Research Manager, Foundational Sciences Focus Area (ENIGMA)  
2007-Now Adjunct Professor, Department of Bioengineering, UC Berkeley, Berkeley CA  
2007-Now Vice President for Technology, the Joint BioEnergy Institute, Berkeley CA  
2005-Now Senior Scientist, Lawrence Berkeley Laboratory, Berkeley CA  
2010-2015 Deputy Division Director, Physical Biosciences, Lawrence Berkeley Laboratory  
2004-2011 Head, Berkeley Center for Structural Biology, Berkeley CA  
2009-2010 Acting Division Director, Physical Biosciences, Lawrence Berkeley Laboratory  
2007-2009 Deputy Division Director, Physical Biosciences, Lawrence Berkeley Laboratory  
2003-2007 Deputy Principal Investigator, Berkeley Structural Genomics Center, Berkeley CA  
1999-2005 Staff Scientist, Lawrence Berkeley Laboratory, Berkeley CA  
1998-1999 Senior Associate, Howard Hughes Medical Institute, New Haven CT  
1998-1999 Research Scientist, Yale University, New Haven CT  
1997-1998 Associate Research Scientist, Yale University, New Haven CT  
1992-1997 Postdoctoral Associate, Yale University, New Haven CT  
1992 Project Scientist, Edinburgh Parallel Computing Center, Edinburgh, Scotland

### **Education**

1988-1992 Ph.D. (Structural analysis and molecular modelling of  $\alpha_{2u}$ -globulin)  
Edinburgh University, Edinburgh, Scotland & Imperial Chemical Industries, UK  
1985-1988 B.Sc. Biological Sciences (Biochemistry), Edinburgh University, Edinburgh, Scotland  
*Summa Cum Laude*

### **Awards**

- DOE Secretary's Achievement Award, Driving U.S. Competitiveness and Innovations Team (2022)
- Director's Technology Transfer Award, Phenix Software Team (2021)
- DOE Secretary's Achievement Award, National Virtual Biotechnology Laboratory COVID-19 Team (2021)
- Department of Energy, Office of Science, Outstanding Mentor Award, Lawrence Berkeley Laboratory, Berkeley CA (2009)
- Outstanding Performance Award, Lawrence Berkeley Laboratory, Berkeley CA (2004)
- Technology Transfer Award, Lawrence Berkeley Laboratory, Berkeley CA (2002)
- Upjohn prize in Biochemistry, Edinburgh University, Edinburgh, Scotland (1988)
- Science Faculty Bursary, Edinburgh University, Edinburgh, Scotland (1986-1987)

### **Other Professional Activities**

Journal reviewer:

- Acta Crystallographica Sections D and F, Biochemistry, Biophysical Journal, Biopolymers, eLife, IUCr, J. Chem. Inf. and Modeling, J. Mol. Biol., JACS, J. Applied Crystallography, J. Synchrotron Radiation, Molecular Microbiology, Nature, Nature Communications, Nature Machine Intelligence, Nature Methods, Nature Protocols, Nature Structural and Molecular Biology, Protein Science, Proteins, PNAS, Royal Society Philosophical Transactions B, Science, Scientific Data, Structure

*Peer review:*

- Diamond Light Source Macromolecular Crystallography Program Review (2023)
- BioCARS beamline review, Advanced Photon Source (2022)
- Diamond Light Source Beamline Software Architecture Review (2022)
- LCLS Science & Instrumentation Review in Structural Biology (2020)
- EMBL PETRA III beamline review, DESY (2019)
- NIH P30 review panel (2019)
- NIH Early Stage MIRA award review panel (2018)
- Member, LCLS Proposal review panel (2014-2019)
- NCI Intramural Structural Biology Program (2004, 2017)
- LS-CAT beamline review, Advanced Photon Source (2014, 2019)
- Macromolecular Crystallography beamline review, Diamond Synchrotron (2014)
- BioCARS beamline review, Advanced Photon Source (2013)
- EMBL Grenoble Outstation review panel (2013)
- KAUST Office of Competitive Research Funds (2013, 2014)
- Charter Member, NIH Molecular Structure and Function D study section (2011-2015)
- Ad hoc reviewer, NIH R13 grants (2011)
- Singapore National Research Foundation proposals (2011)
- DOE Knowledgebase program (2010)
- NIH Challenge Grants (2009)
- Los Alamos Biofuels LDRD program (2009)
- NCRR P41 special emphasis panel (2008)
- Netherlands Organization for Scientific Research (2008, 2010, 2014)
- Ad hoc member, NIH Molecular Structure and Function D study section (2008-2010, 2020)
- DOE Small Business Innovation Research proposals (2008)
- Biotechnology & Biological Sciences Research Council, UK (2008, 2009)
- Wellcome Trust awards, UK (2008)
- DOE INCITE program (2007)
- IMCA-CAT 17-ID Experiment End Station Upgrade, APS (2007)

*Advisory panels:*

- Member, Diamond Light Source (UK) Advisory Committee (2021-Present)
- Member, Pacific Northwest Center for Cryo-EM Advisory Committee (2019-Present)
- Chair, RCSB Advisory Committee (2019-Present)
- Member, RBVI Advisory Committee (2016-2017)
- Member, RCSB Advisory Committee (2015-2019)
- Member, wwPDB Advisory Committee (2013-Present)
- Chair, EM Data Bank Advisory Committee (2013-2016)
- Chair, mmCIF/PDBx working group (2012-Present)
- Member, wwPDB X-ray Validation Task Force (2008-Present)
- Member, Oak Ridge National Laboratory Neutron Future Sciences Advisory Panel (2013)
- Member, Argonne National Laboratory Photon Sciences Advisory Committee (2013)
- Member, Diamond Synchrotron Software Advisory Panel (2012)
- Ad hoc member, NAGMS Council (2010)
- Member, Photon Factory International SAC, Life Science Subcommittee (2009)
- Member, UCLA-DOE Institute for Genomics and Proteomics External Advisory Committee (2008)
- Member, NIGMS/NCRR NSLSII advisory panel (2008-2012)
- Member, Protein Information Management System (PIMS) Scientific Advisory Board (2006-2009)

- Chair, NIH Protein Structure Initiative data management committee (2003-2008)
- Member, International structural genomics organization task force on data deposition (2002-2009)

*Teaching:*

- Instructor, UC Berkeley BioE 225 (Biomolecular Structure Determination) (2017-Present)
- Instructor, UC Berkeley BioE 290D (Biomolecular Structure Analysis) (2009-2016)
- UC Berkeley BioE 24 (2015)
- Guest lecturer, UC Berkeley MCB 206 (2014)
- Guest lecturer Stanford Bio207 (Protein Folding and Disease) (2009, 2010)
- Co-taught UC Berkeley Chem 272A/B (Biomolecular Crystallography) (2006-2008)

**Invited Lectures and Workshops**

**2023**

- Brazilian Crystallographic Association Meeting, online participation, November 14<sup>th</sup>.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 16<sup>th</sup>-31<sup>st</sup>.

**2022**

- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 19<sup>th</sup>-25<sup>th</sup>.

**2021**

- Keystone Conference, Frontiers in Cryo-Electron Microscopy, online, February 2<sup>nd</sup>-6<sup>th</sup>.

**2020**

- Cryo-EM Validation in the Age of SARS-CoV-2: Methods, Tools and Applications, online, November 20<sup>th</sup>.
- Structural Biology Seminar Series, University of Colorado Anschutz Medical Campus, Denver, USA, January 28-30<sup>th</sup>.
- wwPDB Single-particle EM Data-management Workshop, Hinxton, United Kingdom, January 23<sup>rd</sup>-26<sup>th</sup>.
- Stanford-SLAC Cryo-EM Center Cryo-EM Modeling Workshop, Stanford, USA, January 15-17<sup>th</sup>.

**2019**

- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 13<sup>th</sup>-30<sup>th</sup>.
- Structural Biology symposium, Zurich University, Zurich, August 21<sup>st</sup>.
- Phenix Workshop, 32<sup>nd</sup> European Crystallographic Meeting, Vienna, Austria, August 18<sup>th</sup>.
- Crystallographic Computing School, Melk, Austria, August 14-17<sup>th</sup>.
- American Crystallographic Association Annual Meeting, Covington, KY, July 20<sup>th</sup>.
- University of Michigan International Cryo-EM data processing workshop, Ann Arbor, MI, USA, June 19-21<sup>st</sup>.
- Stanford-SLAC Cryo-EM Center Modeling Workshop, Stanford, USA, July 10-12<sup>th</sup>.
- School on 3D CryoEM image analysis, Erice, Italy, May 30<sup>th</sup>-June 6<sup>th</sup>.
- Macromolecular Crystallography School, Instituto de Quimica-Fisica, Madrid, Spain, April 22<sup>nd</sup>-26<sup>th</sup>.
- Single Particle Cryo-EM Course, Cold Spring Harbor Laboratory, USA, March 21<sup>st</sup>-24<sup>th</sup>.
- West Coast Structural Biology Workshop, Asilomar, CA, USA, March 17-19<sup>th</sup>.
- DOE/BER Genomic Sciences Contractors meeting, Tyson's Corner, VA, USA, February 25-27<sup>th</sup>.
- Frontiers in Cryo-EM Validation, European Bioinformatics Institute, Hinxton, Cambridge, UK, January 14-15<sup>th</sup>.

**2018**

- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 14<sup>th</sup>-30<sup>th</sup>.
- Advanced Light Source User meeting, LBNL, Berkeley CA, October 2<sup>nd</sup>.
- European Spallation Source Ikon 15 meeting, Lund University, Lund, Sweden, September 10-12<sup>th</sup>.
- Phenix workshop, Tsinghua University, Beijing, China, September 3-6<sup>th</sup>.
- APS Upgrade Macromolecular Crystallography Workshop, Argonne National Laboratory, IL, USA, August 19-21<sup>st</sup>.

- Cryo-EM workshop, Stockholm, Sweden, August 13-17<sup>th</sup>.
- Phenix Low Resolution Structure Solution Workshop, Technical University of Vienna, Vienna, May 29<sup>th</sup>.
- Modern Concepts in Structural Biology Seminar, Technical University of Vienna, Vienna, May 28<sup>th</sup>.
- Macromolecular Crystallography School, Instituto de Quimica-Fisica, Madrid, Spain, May 3<sup>rd</sup>-11<sup>th</sup>.
- Tsinghua International Symposium of Computational Structural Biology and Biophysics, Beijing, China, April 17<sup>th</sup>-22<sup>nd</sup>.
- 3rd International Symposium on Cryo-3D Image Analysis, Lake Tahoe, USA, March 21<sup>st</sup>-24<sup>th</sup>.
- Single Particle Cryo-EM Course, Cold Spring Harbor Laboratory, USA, March 9<sup>th</sup>-12<sup>th</sup>.

## 2017

- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 26<sup>th</sup>-31<sup>st</sup>.
- American Crystallographic Association Annual Meeting, New Orleans, LA, May 27-29<sup>th</sup>.
- Macromolecular Crystallography School, Instituto de Quimica-Fisica, Madrid, Spain, May 3<sup>rd</sup>-11<sup>th</sup>.
- CCP-EM Spring Symposium, Diamond Light Source, Harwell, United Kingdom, April 24<sup>th</sup>-26<sup>th</sup>.
- DOE/BER Advisory Council meeting, Gaithersburg MD, USA, April 19-21<sup>th</sup>.
- West Coast Protein Crystallography Workshop, Asilomar, USA, March 14<sup>th</sup>-16<sup>th</sup>.

## 2016

- SBGrid/NE-CAT Phenix workshop, Boston, MA, November 9-11<sup>th</sup>.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 21<sup>st</sup>-25<sup>th</sup>.
- DOE/BER Molecules to Mesoscale workshop, Rockville, MD, September 20<sup>th</sup>-23<sup>rd</sup>.
- 12<sup>th</sup> International Conference on Biology and Synchrotron Radiation, Palo Alto, CA, August 22<sup>nd</sup>-24<sup>th</sup>.
- 5<sup>th</sup> International Symposium on Diffraction Structural Biology, Knoxville, TN, August 7-9<sup>th</sup>.
- American Crystallographic Association Annual Meeting, Denver, CO, July 25-26<sup>th</sup>.
- Diffraction Methods in Structural Biology Gordon Conference, Lewiston, ME, July 17<sup>th</sup>-22<sup>nd</sup>.
- Macromolecular Crystallography School, Instituto de Quimica-Fisica, Madrid, Spain, May 19<sup>th</sup>-23<sup>rd</sup>.
- Phenix workshop, Tsinghua University, Beijing, China, May 6-12<sup>th</sup>.
- Phenix workshop, EPFL, Lausanne, Switzerland, February 19-24<sup>th</sup>.
- BioStruct-X Workshop on Ensemble Refinement, Lisbon, Portugal, January 29<sup>th</sup>-February 4<sup>th</sup>.
- Nanomedicine Symposium on Basic & Translational Sciences, MD Anderson, Houston, USA January 27-28<sup>th</sup>.
- Phenix workshop, Shanghai University, Shanghai, China, January 12-18<sup>th</sup>.
- CCP4 Study weekend, Nottingham, UK, January 7-11<sup>th</sup>.

## 2015

- Bay Area Cryo-EM meeting, Berkeley, California, USA, December 4<sup>th</sup>.
- wwwPDB X-ray Validation Task Force Meeting, Cambridge, UK, November 12-18<sup>th</sup>.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 23-27<sup>th</sup>.
- Phenix Workshop, Kansas University, Lawrence Kansas, USA, August 5-7<sup>th</sup>.
- 3D Electron Microscopy Gordon Conference, New London, NH, June 21<sup>st</sup>-26<sup>th</sup>.
- Canadian Light Source Crystallography School, Saskatoon, Canada, June 3<sup>rd</sup>-6<sup>th</sup>.
- Macromolecular Crystallography School, Instituto de Quimica-Fisica, Madrid, Spain, May 19<sup>th</sup>-23<sup>rd</sup>.
- Phenix workshop, Rice University, Houston, USA, April 9-10<sup>th</sup>.

## 2014

- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 24-27<sup>th</sup>.
- mmCIF developers meeting, European Bioinformatics Institute, Hinxton, UK, October 8<sup>th</sup>.
- UC Berkeley BioE Departmental Seminar, Berkeley, CA, USA, September 17<sup>th</sup>.

- BioXFEL workshop, Berkeley, CA, USA, August 21<sup>st</sup>.
- CCP4/NIH workshop, Argonne National Laboratory, USA, June 27<sup>th</sup>-July 1<sup>st</sup>.
- Advanced Methods in Crystallography, Melbourne, Australia June 17-25<sup>th</sup>.
- Phenix workshop, Harvard University, Boston, USA, June 7<sup>th</sup>.
- Macromolecular Crystallography School, Instituto de Quimica-Fisica, Madrid, Spain, May 27<sup>th</sup>-30<sup>th</sup>.
- Mid Atlantic Crystallography meeting/SERCAT Phenix Workshop, U. Maryland, Maryland, USA, April 26<sup>th</sup>.
- University of Lincoln Nebraska Departmental Seminar, Lincoln Nebraska, USA, April 8<sup>th</sup>.
- Recent trends in Macromolecular Structure and Function, Chennai, India, January 22<sup>nd</sup>-25<sup>th</sup>.
- Phenix workshop, Madras University, Chennai, India, January 21<sup>st</sup>.

### **2013**

- NMR/mmCIF developers meeting, European Bioinformatics Institute, Hinxton, UK, November 18<sup>th</sup>-21<sup>st</sup>.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 25<sup>th</sup>-29<sup>th</sup>.
- Theoretical Model Validation Symposium, Rutgers University, USA, October 21<sup>st</sup>-22<sup>nd</sup>.
- International Conference on Structural Genomics, Sapporo, Japan, July 27<sup>th</sup>-August 1<sup>st</sup>.
- CCP4/NIH workshop, Argonne National Laboratory, USA, June 21<sup>st</sup>-25<sup>th</sup>.
- Canadian Light Source Crystallography School, Saskatoon, Canada, June 11-15<sup>th</sup>.
- Joint UCSF/LBNL Imaging Workshop, UCSF, USA, June 7<sup>th</sup>.
- Macromolecular Crystallography School, Instituto de Quimica-Fisica, Madrid, Spain, May 6-13<sup>th</sup>.
- Frontiers in Neutron Structural Biology, Oak Ridge National Laboratory, USA, April 16-18<sup>th</sup>.
- UC Berkeley Structure Supergroup, Berkeley, USA, April 9<sup>th</sup>.
- European Spallation Source, Neutron Protein Crystallography, Aarhus University, Denmark, March 21<sup>st</sup>-22<sup>nd</sup>.

### **2012**

- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 26<sup>th</sup>-November 1<sup>st</sup>.
- New Developments of Methods and Software for Protein Crystallography, Xi'an, China, August 26<sup>th</sup>-28<sup>th</sup>.
- Phenix workshop, Harvard Medical School, Boston, USA, July 27<sup>th</sup>.
- CCP4/NIH workshop, Argonne National Laboratory, USA, June 23<sup>rd</sup>-26<sup>th</sup>.
- Macromolecular Crystallography School, Instituto de Quimica-Fisica "Rocasolano", Madrid, Spain, May 26<sup>th</sup>-29<sup>th</sup>.
- Phenix workshop, Universidad Nacional Autónoma de México, Mexico City, Mexico, April 17<sup>th</sup>-22<sup>nd</sup>.
- Phenix workshop, UT Austin, Texas, USA, Feb 22<sup>nd</sup>.
- Macromolecular Crystallography Workshop, Australian Synchrotron, Melbourne, Australia, February 9<sup>th</sup>-16<sup>th</sup>.

### **2011**

- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 26<sup>th</sup>-30<sup>th</sup>.
- Phenix workshop, ILL Grenoble, October 21<sup>st</sup>.
- Neutrons in Biology, ILL Grenoble, October 19<sup>th</sup>-20<sup>th</sup>.
- SBGrid Annual Meeting, Harvard Medical School, Boston, USA, June 23<sup>rd</sup>-24<sup>th</sup>.
- CCP4 workshop, Argonne National Laboratory, Illinois, June 12<sup>th</sup>-15<sup>th</sup>.
- Phenix workshop, American Crystallographic Association Annual Meeting, New Orleans, USA, May 28<sup>th</sup>.
- Phenix workshop, Utrecht University, Utrecht, Netherlands, May 22<sup>nd</sup>.
- Canadian Light Source Crystallography School, Saskatoon, Canada, May 16<sup>th</sup>-19<sup>th</sup>.
- Phenix workshop, International Conference on Structural Genomics, Toronto, Canada, May 10<sup>th</sup>.

### **2010**

- BHT Meeting, Queen's University, Kingston, Canada, November 5<sup>th</sup>.

- Departmental Seminar, University of Waterloo, Waterloo, Canada, November 4<sup>th</sup>.
- Departmental Seminar, Sick Children's Hospital, Toronto, Canada, November 3<sup>rd</sup>.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 22<sup>nd</sup>-26<sup>th</sup>.
- SSRL User Meeting, Workshop 8, Stanford, USA, October 20<sup>th</sup>.
- Phenix workshop, Rockefeller University, New York, USA, October 6<sup>th</sup>.
- European Crystallography Meeting, Darmstadt, Germany, August 28<sup>th</sup>-31<sup>st</sup>.
- Canadian Light Source Annual Users Meeting, Saskatoon, Canada, June 17<sup>th</sup>.
- CCP4/NIH workshop, Argonne National Laboratory, USA, June 11<sup>th</sup>-14<sup>th</sup>.
- Phenix workshop, University of Houston, Texas, USA, May 30<sup>th</sup>.
- Bio207 (The Life and Death of Proteins), Stanford University, Palo Alto, USA, April 29<sup>th</sup>.
- Recent trends in Macromolecular Structure and Function, Chennai, India, January 7<sup>th</sup>-14<sup>th</sup>.

## 2009

- NCCR Workshop on Crystallographic Computing with Phenix, ETH, Zurich, Switzerland, December 4<sup>th</sup>.
- XXX, IGBMC, Strasbourg, France, December 3<sup>rd</sup>.
- Phenix Workshop, IGBMC, Strasbourg, France, December 2<sup>nd</sup>.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 23<sup>rd</sup>-27<sup>th</sup>.
- SSRL Summer School, Stanford, USA, September 10<sup>th</sup>.
- American Crystallographic Association Annual Meeting, Toronto, Canada, July 26<sup>th</sup>-30<sup>th</sup>.
- CCP4/NIH workshop, Argonne National Laboratory, USA, June 29<sup>th</sup>-July 2<sup>nd</sup>.
- Mid Atlantic Structural Biology meeting, University of Maryland, Maryland, USA, May 29<sup>th</sup>.
- Quantitative Biology Seminar Series, Los Alamos National Laboratory, USA, May 27<sup>th</sup>.
- Bio207 (The Life and Death of Proteins), Stanford University, Palo Alto, USA, April 29<sup>th</sup>.
- Teach SG workshop, Prague, Czech Republic, April 1<sup>st</sup>-5<sup>th</sup>.
- DOE Genomics:GTL awardees meeting, Bethesda, USA, February 7<sup>th</sup>-11<sup>th</sup>.

## 2008

- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 24<sup>th</sup>-28<sup>th</sup>.
- International Structural Genomics Conference, Oxford, UK, September 21<sup>st</sup>-24<sup>th</sup>.
- International Union of Crystallography Congress, Osaka, Japan, August 23<sup>rd</sup>-28<sup>th</sup>.
- Diffraction Methods in Molecular Biology, Gordon Research Conference, Lewiston, Maine, USA, July 13-18<sup>th</sup>.
- Macromolecular Crystallography Course, Beijing, China, May 10<sup>th</sup>-15<sup>th</sup>.
- New Validation Tools for the Macromolecular Crystallography, Cambridge, UK, April 14<sup>th</sup>-16<sup>th</sup>.
- Pittsburgh Conference, New Orleans, USA, March 4<sup>th</sup>-5<sup>th</sup>.
- Recent trends in Macromolecular Structure and Function, Chennai, India, January 7<sup>th</sup>-14<sup>th</sup>.

## 2007

- 16<sup>th</sup> CoLuAa meeting, Aarhus, Denmark, November 9<sup>th</sup>.
- X-ray Crystallography Computing Workshop, Aarhus, Denmark, November 7<sup>th</sup>-8<sup>th</sup>.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 26<sup>th</sup>-30<sup>th</sup>.
- RapiData course, Brookhaven National Laboratory, Brookhaven, USA, April XXXX.
- CCP4/MAX-INF Workshop on Phasing and Refinement, York University, UK, April XXXX.
- The Molecular Replacement method, CCP4 Study Weekend, University of Reading, UK, January XXXX.

## 2006

- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 26<sup>th</sup>-31<sup>st</sup>.

- International Conference on Structural Genomics workshop, Yokohama, Japan, October 19<sup>th</sup>-20<sup>th</sup>.
- Distributed Data Analysis for Neutron Scattering Experiments (DANSE) meeting, Caltech, USA, Aug 15<sup>th</sup>-16<sup>th</sup>.
- European Crystallography Meeting, Leuven, Belgium, August 9<sup>th</sup>-10<sup>th</sup>.
- Neutron Diffraction Workshop, American Crystallographic Association Annual Meeting, Honolulu, Hawaii, USA, August 22<sup>nd</sup>-26<sup>th</sup>.
- Canadian Light Source 9<sup>th</sup> Annual Users Meeting, Saskatoon, Canada, June 15<sup>th</sup>-17<sup>th</sup>.
- 8th International School on the Crystallography of Biological Macromolecules, Como, Italy, May 21<sup>st</sup>-25<sup>th</sup>.
- CCP4/MAX-INF Workshop on Phasing and Refinement, Barcelona, Spain, March 1<sup>st</sup>-7<sup>th</sup>.
- Trends in Macromolecular Structure and Function, Chennai, India, January 18<sup>th</sup>-20<sup>th</sup>.

## 2005

- EMBL M2M Practical Course, EMBL Hamburg, Germany, November 9<sup>th</sup>-15<sup>th</sup>.
- Get Phases workshop, Peking University, Beijing, China, October 29<sup>th</sup>-November 4<sup>th</sup>.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 20<sup>th</sup>-24<sup>th</sup>.
- NCCR Practical Course, Swiss Light Source, Villigen, Switzerland, October 3<sup>rd</sup>-7<sup>th</sup>.
- SSRL Summer School, Stanford, USA, September 13-15<sup>th</sup>.
- 12<sup>th</sup> Northern Protein Structural Workshop, Galashiels, Scotland, September 7<sup>th</sup>-9<sup>th</sup>.
- EMBO Anomalous Diffraction Workshop, ESRF, Grenoble, France, June 15<sup>th</sup>-22<sup>nd</sup>.
- American Crystallographic Association Annual Meeting, Orlando, Florida, USA, May 28<sup>th</sup>-June 1<sup>st</sup>.
- Evolving Methods in Crystallography, Erice, Italy, May 11<sup>th</sup>-22<sup>nd</sup>.
- Data management for high-throughput crystallography, Cambridge University, Cambridge, UK, Feb 9<sup>th</sup>-11<sup>th</sup>.

## 2004

- American Crystallographic Association mmCIF workshop, CARB, Gaithersburg, Maryland, USA, Nov 16<sup>th</sup>.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 30<sup>th</sup>-Nov 2<sup>nd</sup>.
- NIH Protein Structure Initiative Advisory Committee meeting, NIH, Bethesda, USA, October 28<sup>th</sup>.
- ALS Users Meeting, Macromolecular Crystallography Workshop, USA, October 19<sup>th</sup>.
- SSRL Summer School, Stanford, USA, August 16-20<sup>th</sup>.
- EMBO course on Automated Macromolecular Structure Solution, Amsterdam, Netherlands, May 23<sup>rd</sup>-Jun 2<sup>nd</sup>.

## 2003

- UC Berkeley department of Bio-engineering colloquium talk, Berkeley, December 18<sup>th</sup>.
- NIH Protein Structure Initiative Advisory Committee meeting, NIH, Bethesda, USA, December 2<sup>nd</sup>.
- Frontiers in Structural Biology – the Western Canadian Structural Biology Workshop, Banff, Canada, November 21<sup>st</sup>-23<sup>rd</sup>.
- SSRL Summer School, Stanford, USA, September 16-19<sup>th</sup>.
- Aminoff Symposium, Royal Swedish Academy of Sciences, Stockholm, Sweden, September 11-12<sup>th</sup>.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 25<sup>th</sup>-30<sup>th</sup>.
- American Crystallographic Association Annual Meeting, Covington, Kentucky, USA, July 26-30<sup>th</sup>.
- NIH Data Management Workshop, NIH, Bethesda, Maryland, USA, July 10-11<sup>th</sup>.
- EMBO Anomalous Diffraction Workshop, ESRF, Grenoble, France, June 17-23<sup>rd</sup>.
- International Symposium on Diffraction Structural Biology, Tsukuba, Japan, May 28<sup>th</sup>-31<sup>st</sup>.
- Data management aspects of high-throughput structure determination, European Bioinformatics Institute, Hinxton, UK, March 14<sup>th</sup>-15<sup>th</sup>.

## 2002

- Getting the most from biological data: bridging the gap between experiment, analysis and simulation, LBNL offices, Washington DC, December 13<sup>th</sup>.
- Automation for High Throughput Structure Determination, Lawrence Berkeley Laboratory, USA, Dec 6<sup>th</sup>-8<sup>th</sup>.
- High-throughput Synchrotron Crystallography, Argonne National Laboratory, USA, November 20<sup>th</sup>-22<sup>nd</sup>.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 25<sup>th</sup>-28<sup>th</sup>.
- Automation of X-ray Structure Determination for Structural Genomics, Berlin, Germany, October 8<sup>th</sup>-9<sup>th</sup>.
- Diffraction Methods in Molecular Biology, Gordon Research Conference, New London, Connecticut, USA, July 14-19<sup>th</sup>.
- Berkeley & Stanford Synchrotron Radiation Summer School, Stanford, USA, July 8-12<sup>th</sup>.
- Structural Genomics Informatics and Software Integration Workshop, San Antonio, USA, May 22<sup>nd</sup>-23<sup>rd</sup>.
- EMBO Course on Automated Macromolecular Structure Solution, Heidelberg, Germany, May 7-16<sup>th</sup>.
- Interdisciplinary workshop promoting collaboration in high-throughput X-ray structure determination, Santa Fe, USA, March 22-23<sup>rd</sup>.
- High-throughput structure determination, CCP4 Study Weekend, University of York, UK, January 4-5<sup>th</sup>.

## **2001**

- Polarizability in Biomolecular Simulations, Utah, USA, December 13<sup>th</sup>-14<sup>th</sup>.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 19<sup>th</sup>-21<sup>st</sup>.
- ALS Users Meeting, Macromolecular Crystallography Workshop, USA, October 16<sup>th</sup>.
- EMBO/MAX-INF Anomalous Diffraction Workshop, ESRF, Grenoble, France, June 18-23<sup>rd</sup>.
- West Coast Protein Crystallography Workshop, Asilomar, USA, March 25<sup>th</sup>-28<sup>th</sup>.
- ESRF High-throughput workshop, ESRF, Grenoble, France, February 20-21<sup>st</sup>.
- CCP4 Workshop on Refinement of Macromolecular Structure, York University, UK, January 3-9<sup>th</sup>.

## **2000**

- Computational methods in structural biology, Florida State University, Tallahassee, USA, December 5<sup>th</sup>.
- SCBMB seminar, Baylor College of Medicine, Houston, USA, November 6<sup>th</sup>.
- RTG Student Seminar, Arizona State University, Tempe, USA, November 16<sup>th</sup>.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 21-23<sup>rd</sup>.
- SSRL Summer School, Stanford, USA, September 18-23<sup>rd</sup>.
- Diffraction Methods in Molecular Biology, Gordon Research Conference, Andover New Hampshire, USA, July 2-7<sup>th</sup>.
- EMBO workshop for automated macromolecular structure solution, EMBL, Grenoble, France, Mar 15-25<sup>th</sup>.
- CNS workshop, Uppsala University, Uppsala, Sweden, February 7-8<sup>th</sup>.

## **1999**

- High-throughput methods for structural genomics, Argonne National Lab, USA, November 15-16<sup>th</sup>.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 25-27<sup>th</sup>.
- International School of Crystallography of Biological Macromolecules, Barcelona, Spain, September 9-15<sup>th</sup>.
- IUCr Crystallographic Computing School, Cambridge, UK, August 14-20<sup>th</sup>.
- XVIIIth IUCr Congress and General Assembly, Glasgow, UK, August 4-13<sup>th</sup>.
- ACA Summer Course in Crystallography, University of Georgia, USA July 12-24<sup>th</sup>.
- Automation of Structure Determination workshop, Brookhaven National Lab, USA, June 20-21<sup>st</sup>.
- 29th Mid-Atlantic Protein Crystallography Workshop, Rockville, USA, April 28-30<sup>th</sup>.
- CNS Workshop, University of Georgia, USA, April 21<sup>st</sup>.

## **1998**



- EC and CCP4 Workshop on Refinement of Macromolecular Structure, York University, UK, Dec 14-20<sup>th</sup>.
- Advanced School of Macromolecular Crystallography, Sao Carlos, Brazil, November 29<sup>th</sup>-December 6<sup>th</sup>.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 25-27<sup>th</sup>.
- Diffraction Methods in Molecular Biology, Gordon Research Conference, Andover New Hampshire, USA, June 21-26<sup>th</sup>.
- Modelling and membrane proteins, Biochemical Society UK Spring Meeting, Southampton, UK, March 31<sup>st</sup>.

### **1997**

- CCP4 Refinement and Validation Workshop, York University, UK, September 1-6<sup>th</sup>.
- Validation and Refinement of Macromolecular Structures, Oporto, Portugal, August 29-30<sup>th</sup>.
- Modelling of Membrane Proteins, University of Toronto, Canada, May 5<sup>th</sup>.
- West Coast Crystallography Workshop, Asilomar, USA, March 15-18<sup>th</sup>.

### **Prior to 1997**

- Macromolecular Refinement, CCP4 Study Weekend, Chester College, Chester, UK, January 5-6<sup>th</sup> (1996).
- IMA Program on Protein Structure and Dynamics, University of Minnesota, Minnesota, July 18-22<sup>nd</sup> (1994).
- CECAM Workshop on Simulations of biological macromolecules: improving sampling with parallelism and other techniques. Orsay, Paris, November 15-17<sup>th</sup> (1993).

### **Meetings Organized**

#### **2022**

- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 15<sup>th</sup>-31<sup>st</sup>. [Course co-organizer]

#### **2022**

- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 9<sup>th</sup>-25<sup>th</sup>. [Course co-organizer]
- Imaging the rhizosphere and cellular organization, online, January 26-27<sup>th</sup>. [Workshop co-organizer]

#### **2021**

- Intracellular organization, and material synthesis and decomposition, online, December 15-16<sup>th</sup>. [Workshop co-organizer]
- Molecular structures, online, October 27-28<sup>th</sup>. [Workshop co-organizer]

#### **2019**

- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 14<sup>th</sup>-30<sup>th</sup>. [Course co-organizer]

#### **2018**

- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 14<sup>th</sup>-30<sup>th</sup>. [Course co-organizer]

#### **2017**

- Cryo-EM model challenge, Stanford, CA, USA, October 6-8<sup>th</sup>. [Meeting co-organizer]
- Understanding Biology through Structure, Santa Fe, NM, USA, May 13-15<sup>th</sup>. [Session chair]
- Joint BSSD/ASCR session at the DOE/BER Genomic Sciences Contractors Meeting, Arlington, VA, February 7<sup>th</sup>. [Session co-chair]

#### **2016**

- DOE/BER Molecules to Mesoscale workshop, Rockville, MD, September 20<sup>th</sup>-23<sup>rd</sup>. [Meeting co-chair]

#### **2015**

- wwPDB Ligand Validation Workshop, Rutgers University, July 29-31<sup>st</sup>. [Session co-chair]
- EM Modeling Challenge Advisory meeting, MIT, Boston, June 19<sup>th</sup>-21<sup>st</sup>. [Meeting co-organizer]

## 2014

- Hybrid methods workshop, European Bioinformatics Institute, Hinxton, UK, October 6-7<sup>th</sup>. [Session co-chair]
- Soft X-ray sciences workshop, Advanced Light Source, Berkeley, CA, USA, October 1<sup>st</sup>-3<sup>rd</sup>. [Session co-chair]
- Diffraction Methods in Molecular Biology, Gordon Research Conference, Lewiston, Maine, USA, July 27<sup>th</sup> August 1<sup>st</sup>. [Session chair]
- Recent trends in Macromolecular Structure and Function, Chennai, India, January 22<sup>nd</sup>-25<sup>th</sup>. [Member, organizing committee]

## 2013

- International Conference on Structural Genomics, Sapporo, Japan, July 27<sup>th</sup>-August 1<sup>st</sup>. [Session co-chair]

## 2012

- Diffraction Methods in Molecular Biology, Gordon Research Conference, Lewiston, Maine, USA, July 15-20<sup>th</sup>. [Session chair]

## 2011

- Computational Methods session, International Union of Crystallography Meeting, Madrid, Spain, August 22-30<sup>th</sup>. [Session co-chair]
- Phenix Workshop, American Crystallographic Association Annual Meeting, New Orleans, USA, May 28<sup>th</sup>. [Session organizer]
- Phenix Workshop, International Conference on Structural Genomics, Toronto, Canada, May 10<sup>th</sup>. [Session co-organizer]

## 2010

- Diffraction Methods in Molecular Biology, Gordon Research Conference, Lewiston, Maine, USA, July 18-23<sup>rd</sup>. [Session chair]

## 2008

- Pittsburgh Diffraction Conference, Pittsburgh, USA, October 30<sup>th</sup> - November 1<sup>st</sup>. [Session co-organizer]
- Recent trends in Macromolecular Structure and Function, Chennai, India, January 7<sup>th</sup>-14<sup>th</sup>. [Member, organizing committee]

## 2007

- International Symposium on Diffraction Structural Biology, Tokyo, Japan, September 10<sup>th</sup>-13<sup>th</sup>. [Member, international advisory committee]
- Computational Methods Session, American Crystallographic Association Annual Meeting, Salt Lake City, Utah, USA, July 23<sup>rd</sup>-26<sup>th</sup>. [Session co-organizer]
- Multiscale Imaging Workshop, Lawrence Berkeley Laboratory, Berkeley USA, May 17<sup>th</sup>-18<sup>th</sup>. [Meeting co-organizer]

## 2006

- International Conference on Structural Genomics workshop, Yokohama, Japan, October 19<sup>th</sup>-20<sup>th</sup>. [Meeting co-organizer]
- Neutron Diffraction Workshop, American Crystallographic Association Annual Meeting, Honolulu, Hawaii, USA, August 22-26<sup>th</sup>. [Session co-organizer]
- Diffraction Methods in Molecular Biology, Gordon Research Conference, Lewiston, Maine, USA, July 11-16<sup>th</sup>. [Meeting organizer]

## 2004

- Computational Methods Session, American Crystallographic Association Annual Meeting, Chicago, Illinois, USA, July 17-23<sup>rd</sup>. [Session co-organizer]
- Diffraction Methods in Molecular Biology, Gordon Research Conference, Lewiston, Maine, USA, July 11-16<sup>th</sup>. [Meeting co-organizer]

**2003**

- NIH Data Management Workshop, NIH, Bethesda, Maryland, USA, July 10-11<sup>th</sup>. [Meeting co-organizer]

**2002**

- Automation for High Throughput Structure Determination, Lawrence Berkeley Laboratory, USA, December 6<sup>th</sup>-8<sup>th</sup>. [Meeting co-organizer]
- Interdisciplinary workshop promoting collaboration in high-throughput X-ray structure determination, Santa Fe, USA, March 22-23<sup>rd</sup>. [Meeting co-organizer]

**Peer reviewed publications (313 total)**

1. Terwilliger TC, Liebschner D, Croll TI, Williams CJ, McCoy AJ, Poon BK, Afonine PV, Oeffner RD, Richardson JS, Read RJ, Adams PD: AlphaFold predictions are valuable hypotheses and accelerate but do not replace experimental structure determination. *Nature Methods* 2023, online ahead of print.
2. Liebschner D, Afonine PV, Poon BK, Moriarty NW, Adams PD: Improved joint X-ray and neutron refinement procedure in Phenix. *Acta Cryst.* 2023, **D79**:1079-1093.
3. Shrestha S, Awasthi D, Chen Y, Gin J, Petzold CJ, Adams PD, Simmons BA, Singer SW: Simultaneous carbon catabolite repression governs sugar and aromatic co-utilization in *Pseudomonas putida* M2. *Appl Environ Microbiol.* 2023, **89**:e0085223.
4. Afonine PV, Sobolev OV, Moriarty NW, Terwilliger TC, Adams PD: Overall protein structure quality assessment using hydrogen-bonding parameters. *Acta Cryst.* 2023, **D79**:684-693.
5. Chen Y, Gin JW, Wang Y, de Raad M, Tan S, Hillson NJ, Northen TR, Adams PD, Petzold CJ: Alkaline-SDS cell lysis of microbes with acetone protein precipitation for proteomic sample preparation in 96-well plate format. *PLoS One* 2023, **18**:e0288102.
6. Takasuka T, Kim H, Deng K, Bianchetti CM, Yamashita K, Beebe ET, Bergeman LF, Vander Meulen KA, Deutsch S, Ralph J, Adams PD, Northen TR, Fox BG: Quantitative analysis of The High Yield Hydrolysis of Kelp by Laminarinase and Alginate Lyase. *Chembiochem* 2023, **24**:e202300357.
7. Ha NS, Onley JR, Deng K, Andeer P, Bowen BP, Gupta K, Kim PW, Kuch N, Kutschke M, Parker A, Song F, Fox B, Adams PD, de Raad M, Northen TR: A combinatorial droplet microfluidic device integrated with mass spectrometry for enzyme screening. *Lab Chip* 2023, **23**:3361-3369
8. Afonine PV, Adams PD, Urzhumtsev AG: Efficient structure-factor modeling for crystals with multiple components. *Acta Cryst.* 2023, **A79**:345-352.
9. Bhowmick A, Hussein R, Bogacz I, Simon PS, Ibrahim M, Chatterjee R, Doyle MD, Cheah MH, Fransson T, Chernev P, Kim IS, Makita H, Dasgupta M, Kaminsky CJ, Zhang M, Gätcke J, Haupt S, Nangca II, Keable SM, Aydin AO, Tono K, Owada S, Gee LB, Fuller FD, Batyuk A, Alonso-Mori R, Holton JM, Paley DW, Moriarty NW, Mamedov F, Adams PD, Brewster AS, Dobbek H, Sauter NK, Bergmann U, Zouni A, Messinger J, Kern J, Yano J, Yachandra VK: Structural evidence for intermediates during O<sub>2</sub> formation in photosystem II. *Nature* 2023, **617**:629-636.
10. Huang J, Quest A, Cruz-Morales P, Deng K, Pereira JH, Van Cura D, Kakumanu R, Baidoo EEK, Dan Q, Chen Y, Petzold CJ, Northen TR, Adams PD, Clark DS, Balskus EP, Hartwig JF, Mukhopadhyay A, Keasling JD: Complete integration of carbene-transfer chemistry into biosynthesis. *Nature* 2023, **617**:403-408.
11. Englund E, Schmidt M, Nava AA, Lechner A, Deng K, Jovic R, Lin Y, Roberts J, Benites VT, Kakumanu R, Gin JW, Chen Y, Liu Y, Petzold CJ, Baidoo EEK, Northen TR, Adams PD, Katz L, Yuzawa S, Keasling JD: Expanding Extender Substrate Selection for Unnatural Polyketide Biosynthesis by Acyltransferase Domain Exchange within a Modular Polyketide Synthase. *J Am Chem Soc.* 2023. **145**:8822-8832.
12. Sanders BC, Pokhrel S, Labbe AD, Mathews II, Cooper CJ, Davidson RB, Phillips G, Weiss KL, Zhang Q, O'Neill H, Kaur M, Schmidt JG, Reichard W, Surendranathan S, Parvathareddy J, Phillips L, Rainville C, Sterner DE, Kumaran D, Andi B, Babnigg G, Moriarty NW, Adams PD, Joachimiak A, Hurst BL, Kumar S, Butt TR,

- Jonsson CB, Ferrins L, Wakatsuki S, Galanie S, Head MS, Parks JM: Potent and selective covalent inhibition of the papain-like protease from SARS-CoV-2. *Nat Commun.* 2023 **14**:1733.
13. Terwilliger TC, Afonine PV, Liebschner D, Croll TI, McCoy AJ, Oeffner RD, Williams CJ, Poon BK, Richardson JS, Read RJ, Adams PD: Accelerating crystal structure determination with iterative AlphaFold prediction. *Acta Cryst.* 2023, **D79**:234-244.
  14. Prabhakar PK, Pereira JH, Taujale R, Shao W, Bharadwaj VS, Chapla D, Yang JY, Bomble YJ, Moremen KW, Kannan N, Hammel M, Adams PD, Scheller HV, Urbanowicz BR: Structural and biochemical insight into a modular  $\beta$ -1,4-galactan synthase in plants. *Nature Plants* 2023, **9**:486-500.
  15. Dai J, Wilhelm KB, Bischoff AJ, Pereira JH, Dedeo MT, García-Almedina DM, Adams PD, Groves JT, Francis MB: A Membrane-Associated Light-Harvesting Model is Enabled by Functionalized Assemblies of Gene-Doubled TMV Proteins. *Small* 2023, **19**:e2207805.
  16. Liebschner D, Moriarty NW, Poon BK, Adams PD: In situ ligand restraints from quantum-mechanical methods. *Acta Cryst.* 2023, **D79**:100-110
  17. Bloomer BJ, Natoli SN, Garcia-Borràs M, Pereira JH, Hu DB, Adams PD, Houk KN, Clark DS, Hartwig JF: Mechanistic and structural characterization of an iridium-containing cytochrome reveals kinetically relevant cofactor dynamics. *Nature Catalysis* 2023, **6**:39-51
  18. Deng K, Wang X, Ing N, Opgenorth P, de Raad M, Kim J, Simmons BA, Adams PD, Singh AK, Lee TS, Northen TR: Rapid quantification of alcohol production in microorganisms based on nanostructure-initiator mass spectrometry (NIMS) *Anal. Biochem.* 2023, **662**:114997
  19. Tom LM, Aulitto M, Wu YW, Deng K, Gao Y, Xiao N, Rodriguez BG, Louime C, Northen TR, Eudes A, Mortimer JC, Adams PD, Scheller HV, Simmons BA, Ceja-Navarro JA, Singer SW: Low-abundance populations distinguish microbiome performance in plant cell wall deconstruction. *Microbiome* 2022 **10**:183
  20. Terwilliger TC, Poon BK, Afonine PV, Schlicksup CJ, Croll TI, Millán C, Richardson JS, Read RJ, Adams PD: Improved AlphaFold modeling with implicit experimental information. *Nat Methods* 2022, **19**:1376-1382
  21. Liu AK, Pereira JH, Kehl AJ, Rosenberg DJ, Orr DJ, Chu SKS, Banda DM, Hammel M, Adams PD, Siegel JB, Shih PM: Structural plasticity enables evolution and innovation of RuBisCO assemblies. *Sci. Adv.* 2022, **8**:eadc9440
  22. Andi B, Kumaran D, Kreitler DF, Soares AS, Keereetaweeep J, Jakoncic J, Lazo EO, Shi W, Fuchs MR, Sweet RM, Shanklin J, Adams PD, Schmidt JG, Head MS, McSweeney S: Hepatitis C virus NS3/4A inhibitors and other drug-like compounds as covalent binders of SARS-CoV-2 main protease. *Sci. Rep.* 2022, **12**:12197
  23. Macdonald SS, Pereira JH, Liu F, Tegl G, DeGiovanni A, Wardman JF, Deutsch S, Yoshikuni Y, Adams PD, Withers SG: A Synthetic Gene Library Yields a Previously Unknown Glycoside Phosphorylase That Degrades and Assembles Poly- $\beta$ -1,3-GlcNAc, Completing the Suite of  $\beta$ -Linked GlcNAc Polysaccharides. *ACS Central Science* 2022, **8**:430-440.
  24. Westbrook JD, Young JY, Shao C, Feng Z, Guranovic V, Lawson CL, Vallat B, Adams PD, Berrisford JM, Bricogne G, Diederichs K, Joosten RP, Keller P, Moriarty NW, Sobolev OV, Velankar S, Vonrhein C, Waterman DG, Kurisu G, Berman HM, Burley SK, Peisach E: PDBx/mmCIF Ecosystem: Foundational Semantic Tools for Structural Biology. *J Mol Biol.* 2022, **434**:167599.
  25. Iwai K, Wehrs M, Garber M, Sustarich J, Washburn L, Costello Z, Kim PW, Ando D, Gaillard WR, Hillson NJ, Adams PD, Mukhopadhyay A, Garcia Martin H, Singh AK: Scalable and automated CRISPR-based strain engineering using droplet microfluidics. *Microsyst Nanoeng.* 2022, **8**:31.
  26. Chen Y, Kaplan Lease N, Gin JW, Ogorzalek TL, Adams PD, Hillson NJ, Petzold CJ: Modular automated bottom-up proteomic sample preparation for high-throughput applications. *PLoS One* 2022, **17**:e0264467.
  27. Hancock M, Peulen TO, Webb B, Poon B, Fraser JS, Adams P, Sali A: Integration of software tools for integrative modeling of biomolecular systems. *J. Struct. Biol.* 2022, **214**:107841.

28. Hussein R, Ibrahim M, Bhowmick A, Simon PS, Chatterjee R, Lassalle L, Doyle M, Bogacz I, Kim IS, Cheah MH, Gul S, de Lichtenberg C, Chernev P, Pham CC, Young ID, Carbajo S, Fuller FD, Alonso-Mori R, Batyuk A, Sutherlin KD, Brewster AS, Bolotovskiy R, Mendez D, Holton JM, Moriarty NW, Adams PD, Bergmann U, Sauter NK, Dobbek H, Messinger J, Zouni A, Kern J, Yachandra VK, Yano J: Structural dynamics in the water and proton channels of photosystem II during the S2 to S3 transition. *Nature Communications* 2021, **12**:6531.
29. Baek M, DiMaio F, Anishchenko I, Dauparas J, Ovchinnikov S, Lee GR, Wang J, Cong Q, Kinch LN, Schaeffer RD, Millán C, Park H, Adams C, Glassman CR, DeGiovanni A, Pereira JH, Rodrigues AV, van Dijk AA, Ebrecht AC, Opperman DJ, Sagmeister T, Buhlheller C, Pavkov-Keller T, Rathinaswamy MK, Dalwadi U, Yip CK, Burke JE, Garcia KC, Grishin NV, Adams PD, Read RJ, Baker D: Accurate prediction of protein structures and interactions using a three-track neural network. *Science* 2021, **373**:871-876
30. Ibrahim M, Moriarty NW, Kern J, Holton JM, Brewster AS, Bhowmick A, Bergmann U, Zouni A, Messinger J, Yachandra VK, Yano J, Dobbek H, Sauter NK, Adams PD: Reply to Wang et al.: Clear evidence of binding of O<sub>x</sub> to the oxygen-evolving complex of photosystem II is best observed in the omit map. *Proc Natl Acad Sci U S A*. 2021 **118**:e2102342118
31. Ing N, Deng K, Chen Y, Aulitto M, Gin JW, Pham TLM, Petzold CJ, Singer SW, Bowen B, Sale KL, Simmons BA, Singh AK, Adams PD, Northen TR: A multiplexed nanostructure-initiator mass spectrometry (NIMS) assay for simultaneously detecting glycosyl hydrolase and lignin modifying enzyme activities. *Sci Rep*. 2021 **11**:11803
32. Pham LTM, Deng K, Northen TR, Singer SW, Adams PD, Simmons BA, Sale KL: Experimental and theoretical insights into the effects of pH on catalysis of bond-cleavage by the lignin peroxidase isozyme H8 from *Phanerochaete chrysosporium*. *Biotechnol Biofuels*. 2021, **14**:108
33. Lui LM, Majumder EL, Smith HJ, Carlson HK, von Netzer F, Fields MW, Stahl DA, Zhou J, Hazen TC, Baliga NS, Adams PD, Arkin AP: Mechanism Across Scales: A Holistic Modeling Framework Integrating Laboratory and Field Studies for Microbial Ecology. *Front Microbiol*. 2021, **12**:642422.
34. Terwilliger TC, Sobolev OV, Afonine PV, Adams PD, Ho CM, Li X, Zhou ZH: Protein identification from electron cryomicroscopy maps by automated model building and side-chain matching. *Acta Cryst*. 2021, **D77**:457-462
35. van Zundert GCP, Moriarty NW, Sobolev OV, Adams PD, Borrelli KW: Macromolecular refinement of X-ray and cryoelectron microscopy structures with Phenix/OPLS3e for improved structure and ligand quality. *Structure* 2021, **29**:913-921.e4
36. Teze D, Coines J, Fredslund F, Dubey KD, Bidart GN, Adams PD, Dueber JE, Svensson B, Rovira C, Welner DH: O-/N-/S-Specificity in Glycosyltransferase Catalysis: From Mechanistic Understanding to Engineering. *ACS Catalysis* 2021, **11**:1810-1815.
37. Kim J, Baidoo EEK, Amer B, Mukhopadhyay A, Adams PD, Simmons BA, Lee TS: Engineering *Saccharomyces cerevisiae* for isoprenol production. *Metab Eng*. 2021, **64**:154-166.
38. Lawson CL, Kryshchuk A, Adams PD, Afonine PV, Baker ML, Barad BA, Bond P, Burnley T, Cao R, Cheng J, Chojnowski G, Cowtan K, Dill KA, DiMaio F, Farrell DP, Fraser JS, Herzik MA Jr, Hoh SW, Hou J, Hung LW, Igaev M, Joseph AP, Kihara D, Kumar D, Mittal S, Monastyrskyy B, Olek M, Palmer CM, Patwardhan A, Perez A, Pfab J, Pintilie GD, Richardson JS, Rosenthal PB, Sarkar D, Schäfer LU, Schmid MF, Schröder GF, Shekhar M, Si D, Singharoy A, Terashi G, Terwilliger TC, Vaiana A, Wang L, Wang Z, Wankowicz SA, Williams CJ, Winn M, Wu T, Yu X, Zhang K, Berman HM, Chiu W: Cryo-EM model validation recommendations based on outcomes of the 2019 EMDDataResource challenge. *Nature Meth*. 2021, **18**:156-164.
39. Wang X, Pereira JH, Tsutakawa S, Fang X, Adams PD, Mukhopadhyay A, Lee TS: Efficient production of oxidized terpenoids via engineering fusion proteins of terpene synthase and cytochrome P450. *Metab. Eng*. 2021, **64**:41-51.

40. Liebschner D, Afonine PV, Moriarty NW, Poon BK, Chen VB, Adams PD: CERES: a cryo-EM re-refinement system for continuous improvement of deposited models. *Acta Cryst.* 2021, **D77**:48-61.
41. Moriarty NW, Liebschner D, Tronrud DE, Adams PD: Arginine off-kilter: guanidinium is not as planar as restraints denote. *Acta Cryst.* 2020, **D76**:1159-1166.
42. Ge X, Thorgersen MP, Poole FL 2nd, Deutschbauer AM, Chandonia JM, Novichkov PS, Gushgari-Doyle S, Lui LM, Nielsen T, Chakraborty R, Adams PD, Arkin AP, Hazen TC, Adams MWW: Characterization of a Metal-Resistant *Bacillus* Strain With a High Molybdate Affinity ModA From Contaminated Sediments at the Oak Ridge Reservation. *Front Microbiol.* 2020, **11**:587127.
43. Ge X, Thorgersen MP, Poole FL 2nd, Deutschbauer AM, Chandonia JM, Novichkov PS, Adams PD, Arkin AP, Hazen TC, Adams MWW: Draft Genome Sequence of *Bacillus* sp. Strain EB106-08-02-XG196, Isolated from High-Nitrate-Contaminated Sediment. *Microbiol Resour Announc.* 2020, **9**:e01149-20.
44. Terwilliger TC, Sobolev OV, Afonine PV, Adams PD, Read RJ: Density modification of cryo-EM maps. *Acta Cryst.* 2020, **D76**:912-925.
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